

Bulk-edge correspondence, spectral flow and Atiyah-Patodi-Singer theorem for the \mathbb{Z}_2 -invariant in topological insulators

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We study the bulk-edge correspondence in topological insulators by taking Fu-Kane spin pumping model as an example. We show that the Kane-Mele invariant in this model is \mathbb{Z}_2 invariant modulo the spectral flow of a single-parameter family of 1+1-dimensional Dirac operators with a global boundary condition induced by the Kramers degeneracy of the system. This spectral flow is defined as an integer which counts the difference between the number of eigenvalues of the Dirac operator family that flow from negative to non-negative and the number of eigenvalues that flow from non-negative to negative. Since the bulk states of the insulator are completely gapped and the ground state is assumed being no more degenerate except the Kramers, they do not contribute to the spectral flow and only edge states contribute to. The parity of the number of the Kramers pairs of gapless edge states is exactly the same as that of the spectral flow. This reveals the origin of the edge-bulk correspondence, i.e., why the edge states can be used to characterize the topological insulators. Furthermore, the spectral flow is related to the reduced η -invariant and thus counts both the discrete ground state degeneracy and the continuous gapless excitations, which distinguishes the topological insulator from the conventional band insulator even if the edge states open a gap due to a strong interaction between edge modes. We emphasize that these results are also valid even for a weak disordered and/or weak interacting system. The higher spectral flow to categorize the higher-dimensional topological insulators are expected.

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I. INTRODUCTIONS

Studies on the topological classification of the new condensed matter systems have greatly enriched the zoo of quantum states of matter [1–3]. Pioneer development in this field was the discovery of the topological nature of the quantum Hall effect which is described by the TKNN topological invariant for a pure system [4] and its generalization to disordered and interacting systems [5, 6].

Recently found topological insulators with time reversal symmetry [7, 8] make the family of the topological quantum matter become very affluent [9–11]. These systems may be robust to the weak disorders and weak interactions [12–18]. Experimentally, these time reversal invariant insulators have been or are possibly realized in quantum wells, alloys and crystals [19–25].

These time reversal invariant systems own a common topological property, i.e., a \mathbb{Z}_2 -valued topological invariant [9, 10], instead of the integer-valued one like the TKNN invariant. We name this \mathbb{Z}_2 -valued topological invariant as Kane-Mele's invariant. Correspondingly, these systems with non-trivial Kane-Mele's invariant are of different edge states from the conventional band insulator: The odd number of the pairs of the gapless edge excitations [9, 10].

On the other hand, the topological insulator can also be characterized by another kind of topological invariant: Descendence to $3 + 1$ - and $2 + 1$ -dimensions from the

Chern-Simons in a $4 + 1$ -dimensional space-time which includes the three-dimensional Brillouin zone [26].

These two different topological invariants are proved being exactly equivalent [27]. In fact, this equivalence gives an index theorem between the topological index which is discrete (i.e., Kane-Mele's here) and an analytic index (i.e., the Chern-Simons and its descendance), similar to the Euler number, which is a topological index defined by the triangulation, is exactly equal to the analytic index given by Gauss-Bonnet theorem. A more relevant index theorem is the index theorem of Dirac operator because the gapless edge excitations of these topological insulators are exactly Dirac-type.

Although the topological invariant defined over the Brillouin zone may nicely reflect the topological property of the quantum space, it is not clear how this topological invariant relates to the topological index of the Dirac operator acting on the quantum space in the real space representation. For the topological p -wave paired superfluid, such a relation has been provided by one of the authors [28]. In the topological insulators, for both with and without the time reversal symmetry, the definition of the topological invariants stemming from the real space lacks.

The bulk-edge correspondence, more generally, the bulk-boundary correspondence, is an essential phenomenon in topological states of matter. This has been known since the integer quantum Hall effects were discov-

ered [29]. Many recent studies focus on this problem [30–38]. There are several expressions of this correspondence according to the problems in various scenarios. Topologically, this is the correspondence between the number of the *real space* gapless edge (boundary) states and the *momentum space* topological invariant. It is a fact but not clear yet why such a correspondence hold. In our opinion, to well understand this correspondence from a topological point of view, Atiyah-Patodi-Singer index theorem [40, 41] for Dirac operator must play a key role.

To study such a correspondence for arbitrary dimensional space-time requires some more mathematical tools that the condensed matter physicists are not familiar. We will gradually introduce to readers these tools in the present work and subsequent works. As the first step, we study the systems with a 1 + 1-dimensional Dirac operator. An example of such a system was provided Fu and Kane [39]. Its lattice version is a one-dimensional tight binding model of electrons with a staggered magnetic field, a staggered bond modulation as well as a time reversal invariant spin-orbit coupling. For this model, Fu and Kane analyzed the \mathbb{Z}_2 adiabatic spin pump between the topological insulating material and a reservoir. The \mathbb{Z}_2 -valued topological invariant in this \mathbb{Z}_2 pump is similar to the \mathbb{Z}_2 topological invariant (Kane-Mele’s invariant) in a two-dimensional topological insulator. In the continuous limit, there is a well-defined Dirac operator in this model. We can show that its spectral problem can be solved with a so-called Atiyah-Patodi-Singer global boundary condition [40, 41], which is induced by the Kramers degeneracy.

With this example in mind, we study a model-independent Atiyah-Patodi-Singer boundary problem for a 1+1-dimensional topological insulator. We show that Kane-Mele’s invariant is \mathbb{Z}_2 -modular to the spectral flow of a single-parameter family of the Dirac operators. Here, the spectral flow is defined as *an integer which counts the difference between the number of eigenvalues of the Dirac operator family that flow from negative to non-negative and the number of eigenvalues that flow from non-negative to negative*. Therefore, Kane-Mele’s invariant is computed by counting the discrete ground state degeneracy and the number of the continuous gapless excitations.

In a pure topological insulator where the Dirac operators can be parameterized by the Brillouin zone, the ground state is assumed to be not degenerate except Kramers degeneracy and thus the parity of the spectral flow is the same as that of the number of the pairs of the gapless edge states. This explains why the edge states can distinguish the topological insulator from the conventional band insulator.

Since the spectrum of the Dirac operators is determined by the topology of the quantum state space based on the real space-time, we can also alter the parametrization other than the Brillouin zone when it is not a convenient one. For a system with disorder or interaction, a well-known parametrization is the twisted boundary

condition [5, 6], whose usage to the 1+1-dimensions [39] and other topological insulator systems [15] have been studied. Thus, our results can also be used to the 1+1-dimensional topological insulator with disorder and weak interaction.

For a strong interaction between the edge states, a gap opens at the edge but the ground state becomes degenerate [12, 13, 39] while the topological nature described by Kane-Mele’s invariant is still kept. There is a theorem that a non-trivial topological invariant may lead to either ground state degeneracy or gapless excitations [14]. From the spectral flow point of view, it is easy to be understood because the spectral flow counts both the discrete ground state degeneracy and the number of the continuous gapless excitations.

The strong interaction between the bulk Dirac particles may modify the \mathbb{Z}_2 topological insulators to \mathbb{Z}_8 ones [42]. Since the Atiyah-Patodi-Singer boundary problem concerns the linear Dirac equation, our result can not be directly applied to the strong interacting topological insulators. More mathematic tools concerning the non-linear Dirac equations are required and this is out of our goal in this paper.

The studies for the 1+1-dimensional topological insulators can be generalized to higher-dimensional space-time but this involves some advanced mathematical tools, e.g., to define a higher spectral flow [43]. We shall sketch the possible generalization and leave the details for the subsequent studies.

This paper is organized as follows: In Sec. II, we introduce the time reversal invariant model with \mathbb{Z}_2 spin pump given by Fu and Kane [39] and its continuous limit. The Atiyah-Patodi-Singer boundary condition problem corresponding to the Kramers degeneracy is set up. In Sec. III, we define the η -invariant and spectral flow [44]. In Sec. IV, we prove a theorem that relates the η -invariant to the boundary projection that is defined by the Atiyah-Patodi-Singer boundary condition. Mathematically, it is the Scott-Wojciechowski theorem [45]. The section V devotes our main result, Kane-Mele’s invariant, a winding number related to the boundary projection, is \mathbb{Z}_2 -modular to the spectral flow of the family of the Dirac operators. In Sec. VI, we generalize the main result to disordered and interacting systems. In Sec. VII, we argue that our result may be generalized to the higher-dimensional space-time. The final section is discussions and conclusions.

II. 1+1-DIMENSIONAL TOPOLOGICAL INSULATOR AND ATIYAH-PATODI-SINGER BOUNDARY PROBLEM

Although the Atiyah-Patodi-Singer boundary problem we shall solve is not dependent on a concrete model, having such a system is helpful to obtain an intuitive understanding. In this section, we first review the 1+1-dimensional topological insulator model with \mathbb{Z}_2 spin

pump proposed by Fu and Kane and Kane-Mele's invariant in this model [39]. In the continuous limit, we obtain a single-parameter family of the Dirac operators in 1+1-dimensional space-time. The first three subsections basically are the summary of those results we will use in this work. With the Kramers degeneracy, we then abstract a model-independent Atiyah-Patodi-Singer boundary problem which is the starting point to show the relation between Kane-Mele's invariant and the spectral flow of the Dirac operator family.

A. Tight Binding Model

Consider a one-dimensional lattice in which electrons are allowed only hopping between the nearest neighbor sites and suffer a staggered magnetic field and a staggered bond modulation as well as a time reversal invariant spin-orbit coupling. Namely, the Hamiltonian of the system is given by

$$H = H_0 + V_h + V_b + V_{so}, \quad (1)$$

where

$$\begin{aligned} H_0 &= -t_0 \sum_{\langle ij \rangle, \alpha} (c_{i\alpha}^\dagger c_{j\alpha} + h.c.), \\ V_h &= h \sum_{i, \alpha\beta} (-1)^i \sigma_{\alpha\beta}^z c_{i\alpha}^\dagger c_{i\beta}, \\ V_b &= b \sum_{\langle ij \rangle, \alpha} (-1)^i (c_{i\alpha}^\dagger c_{j\alpha} + h.c.), \\ V_{so} &= \sum_{\langle ij \rangle, \alpha\beta} i \mathbf{e} \cdot \vec{\sigma}_{\alpha\beta} (c_{i\alpha}^\dagger c_{j\beta} - c_{j\alpha}^\dagger c_{i\beta}), \end{aligned}$$

The last term is the spin-orbital coupling which is characterized by the vector \mathbf{e} and violates the conservation of S_z . Fu and Kane consider an adiabatic cycle as time t varying from 0 to T [39]

$$b(t) = b^0 \cos(2\pi t/T), \quad h(t) = h^0 \sin(2\pi t/T). \quad (2)$$

The Hamiltonian becomes time reversal invariant only at $t = 0$ and $t = T/2$.

The spectrum has been calculated and turns out the existence of a single pair of gapless edge excitations. This characterizes this non-trivial topological insulator.

B. Kane-Mele's Invariant

We assume the one-dimensional lattice has a lattice constant $a = 1$ and the length L with a periodic boundary condition. The $2N$ bands are occupied. A unitary transformation $H(k) = e^{ikx} H e^{-ikx}$ parameterizes the Hamiltonian in the Brillouin zone $-\pi \leq k \leq \pi$. Under a time reversal transformation,

$$\Theta H(-k, -t) \Theta^{-1} = H(k, t), \quad (3)$$

with the time reversal operator

$$\Theta = e^{i\pi S_y} C \quad (4)$$

for S_y is the y -component of the spin operator and C being the complex conjugate. The spectrum is Kramers degenerate at $(k, t) = \{\Gamma_i\} = \{(0, 0), (0, T/2), (\pi, 0), (\pi, T/2)\}$ since $H(k, t)$ is time reversal invariant at these points.

According to the Bloch theorem, the n -band Bloch wave function reads

$$|\psi_{k,n}\rangle = \frac{1}{\sqrt{L}} e^{ikx} |u_{k,n}\rangle \quad (5)$$

where $|u_{k,n}\rangle$ is cell-periodic.

Due to the Kramers degeneracy, the time reversal operator defines a map w from $|u_{k,n}\rangle$ to its Kramers partner $|u_{m,-k}\rangle$, namely,

$$w_{mn} = \langle u_{-k,m} | \Theta | u_{k,n} \rangle \quad (6)$$

In fact, also due to the Kramers degeneracy, the $2N$ bands can be labelled by (α, a) for $\alpha = 1, \dots, N$ and $a = 0, 1$. For a given α , the eigenvalues of the Hamiltonian $E_\alpha^0(-k) = E_\alpha^1(k)$ due to time reversal symmetry. Therefore, up to a $U(1)$ phase, $|u_{-k,\alpha}^0\rangle$ is the Kramers partner of $|u_{k,\alpha}^1\rangle$ [39],

$$\begin{aligned} |u_{-k,\alpha}^0\rangle &= e^{i\chi_{k,\alpha}} \Theta |u_{k,\alpha}^1\rangle, \\ |u_{-k,\alpha}^1\rangle &= -e^{i\chi_{-k,\alpha}} \Theta |u_{k,\alpha}^0\rangle, \\ \langle u_{-k,\alpha}^a | &= (-1)^a \langle u_{k,\alpha}^{a+1} | \Theta^\dagger e^{-i\chi_{(-1)^a k, \alpha}}. \end{aligned} \quad (7)$$

The effective parameter space τ_1 in (k, t) is reduced to the area that is surrounded by the lines linking four time reversal invariant points Γ_i . Kane-Mele's \mathbb{Z}_2 -valued invariant which categorizes this topological insulator is given by

$$\text{wind}(w)_{\partial\tau_1} = \sum_i [\log \sqrt{\det(w(\Gamma_i))} - \log \text{Pf}(w(\Gamma_i))], \quad (8)$$

which is the winding number of the mapping w around the boundary $\partial\tau_1$ of the effective parameter space τ_1 .

C. Continuous Limit

To relate to the Atiyah-Patodi-Singer boundary problem, we go to the continuous limit of the lattice model. The continuous version of (1) is described by the Hamiltonian density [39]

$$\begin{aligned} H &= \psi_{a\alpha}^* (i v_F \tau_{ab}^z \delta_{\alpha\beta} \partial_x + h \tau_{ab}^x \sigma_{\alpha\beta}^z \\ &\quad + b \tau_{ab}^y \delta_{\alpha\beta} + \tau_{ab}^z \mathbf{e} \cdot \vec{\sigma}_{\alpha\beta}) \psi_{b\beta} \end{aligned} \quad (9)$$

where $\psi_{a\alpha}$ is four-component fermion field with $a = L, R$ denoting the left- and right-movings and α being the spin.

τ and σ are Pauli matrices corresponding to a and α , respectively. From this Hamiltonian, we read out an effective Dirac operator

$$D(t) = iv_F \tau^z \sigma^0 \partial_x + h(t) \tau^x \sigma^z + b(t) \tau^y \sigma_0 + \tau^z \mathbf{e} \cdot \vec{\sigma}, \quad (10)$$

where σ^0 is the identity matrix acting on the spin.

D. The Atiyah-Patodi-Singer Boundary Problem

We have presented an example of 1+1-dimensional topological insulator with time reversal invariant. There is a Dirac operator which relates to the gapless edge Dirac cone. Parameterizing the Dirac operator with the Brillouin zone, $D(k, t) = e^{-ikx} D(t) e^{ikx}$, we have a family of the Dirac operators.

For a given Dirac operator in a space-time with a boundary, a local boundary condition is often not allowed [40, 41]. Instead, one has to introduce a global boundary condition on the boundary.

To describe a global boundary condition, we first make some definitions.

(i) Let $\text{Spec} D = \{\lambda\}$ denote all the eigenvalues that obey $D\psi_\lambda = \lambda\psi_\lambda$. We call $\text{Spec} D$ the spectrum of D .

(ii) Let $\text{Spec}_P D = \{\lambda_P\}$ be a subset of $\text{Spec} D$.

(iii) Denote $|\phi_P\rangle = \sum_{\lambda_P} a_{\lambda_P} |\psi_{\lambda_P}\rangle$. Define a projection P so that $P|\phi_P\rangle = 0$ for all $|\phi_P\rangle$.

For a space-time M and its boundary ∂M , a global boundary condition is often given by, for a projection P , $P|\phi_P\rangle|_{\partial M} = 0$.

A general Atiyah-Patodi-Singer boundary problem is to solve the problem $D|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$ with a global boundary condition $P|\phi_P\rangle|_{\partial M} = 0$ for a subset of $\{\lambda_P\}$. For simplicity, we denote the operator D_P the Dirac operator obeying the boundary condition.

For a family of the Dirac operators $D(k)$, we can have a family of the boundary condition problems with $D_{P(k)}$.

The general description of the Atiyah-Patodi-Singer boundary problem is somewhat abstract. We present an example according to the model we are studying in this section. The space-time $\{(x, t)\}$ in the periodic boundary condition is a two-dimensional torus. Due to the Kramers degeneracy, we study a cylinder $M = S^1 \times [0, T/2]$. The boundary of this cylinder is $\partial M = (S^1 \times \{0\}) \cup (S^1 \times \{T/2\})$. For the family of the $D(k)$ with the wave functions $|u_{k,\alpha}^a\rangle$, we define a map $Q(k)$:

$$Q(k)|u_{-k,\alpha}^a\rangle = |u_{k,\alpha}^a\rangle, \quad (11)$$

The Kramers degeneracy related to the time reversal symmetry defines a projection, i.e., we can rewrite (7) as

$$\begin{aligned} P(k) \begin{bmatrix} |u_{-k,\alpha}^0\rangle \\ |u_{-k,\alpha}^1\rangle \end{bmatrix} \\ = \frac{1}{2} \begin{bmatrix} |u_{-k,\alpha}^0\rangle - e^{i\chi_{k,\alpha}} \Theta Q(k) |u_{-k,\alpha}^1\rangle \\ |u_{-k,\alpha}^1\rangle + e^{i\chi_{-k,\alpha}} \Theta Q(k) |u_{-k,\alpha}^0\rangle \end{bmatrix} = 0. \end{aligned} \quad (12)$$

The Atiyah-Patodi-Singer boundary problem is now defined by

$$D(k)\psi(x, t)|_{\partial M} = \lambda(k)\psi(x, t)|_{\partial M} \quad (13)$$

with the global boundary condition

$$P(k)\psi|_{\partial M} = 0. \quad (14)$$

We said the boundary condition (14) is global because the project operator $P(k)$ is dependent on the wave vector k but not locally on the coordinate x .

This is the problem we are going to solve in the rest of this paper. We would like to emphasize that the "boundary condition" (14) in this Atiyah-Patodi-Singer boundary problem is not the real physical boundary condition of the system in which the wave function is periodic both in the spatial and time directions. In the materials, the physical boundary condition may be more different from (14). For example, instead of on the circle S^1 , the one-dimensional lattice in reality is a chain with open boundaries. However, the physical boundary changes do not affect our results as we will argue later. (See Sec. V B.)

III. η -INVARIANT AND SPECTRAL FLOW

As we have introduced, to relate Kane-Mele's invariant to the edge states, one needs to use the concept of the spectral flow. In this section, we define the spectral flow and its analytical expression in the η -invariant. With the notations that are easier to be understood by physicists, this section basically is a review to the definitions and results in Sec. 3 in Ref. [44].

A. η - and ζ -invariants

For the Dirac operator D_P , the η - and ζ -functions are defined, for $\text{Re}(s) \gg 0$, by

$$\begin{aligned} \eta(D_P; s) &= \text{tr}(D_P |D_P|^{-s-1}) = \sum_{\lambda \in \text{Spec}' D_P} \text{sign}(\lambda) |\lambda|^{-s}, \\ \zeta(D_P; s) &= \text{tr}(D_P^{-s}) = \sum_{\lambda \in \text{Spec}' D_P} \lambda^{-s}, \end{aligned} \quad (15)$$

where the prime on $\text{Spec} D$ means the zero eigenvalues of λ are excluded.

For a general P , one has

$$\begin{aligned} \zeta(D_P; s) &= \frac{1}{2} (\zeta(D_P^2; s/2) + \eta(D_P; s)), \\ &+ (-1)^{-s} \frac{1}{2} (\zeta(D_P^2; s/2) - \eta(D_P; s)), \end{aligned} \quad (16)$$

which can be seen by writing the right hand side as

$$\begin{aligned}
& \frac{1}{2} \left[\sum_{\lambda_P > 0} ((\lambda_P^2)^{-s/2} + \lambda_P^{-s}) \right. \\
& + \sum_{\lambda_P < 0} ((|\lambda_P|^2)^{-s/2} - (-1)^{-s} |\lambda_P|^{-s}) \\
& + (-1)^{-s} \frac{1}{2} \left[\sum_{\lambda_P > 0} ((\lambda_P^2)^{-s/2} - \lambda_P^{-s}) \right. \\
& + \sum_{\lambda_P < 0} ((|\lambda_P|^2)^{-s/2} + (-1)^{-s} |\lambda_P|^{-s}) \\
& \left. \left. = \sum_{\lambda_P > 0} \lambda_P^{-s} + \sum_{\lambda_P < 0} (-1)^s |\lambda_P|^{-s} \right] \right]
\end{aligned}$$

The right hand side of the last equality is exactly the definition of $\zeta(D_P; s)$.

For the projection $P = P(k)$ [46], the η - and ζ -functions are regular at $s = 0$. Moreover, $\zeta(D_{P(k)}; 0)$ is not dependent on k .

The η -invariant of D_P is defined by

$$\eta(D_P) = \eta(D_P; 0), \quad (17)$$

which counts the asymmetry between non-zero positive eigen states and non-zero negative eigen states. To include the zero modes, we define so-called *reduced η -invariant*:

$$\tilde{\eta}(D_P) = \frac{1}{2}(\eta(D_P) + \eta_0(D_P)) \quad (18)$$

where $\eta_0(D_P)$ is the number of the independent zero modes.

For a general projection P , a family of $\eta(D_{P(k)})$ does not vary smoothly in the whole interval $k \in [0, \pi]$. However, $\tilde{\eta}(D_{P(k)})$ is smooth [47]. Furthermore, a real-valued function or a k -dependent Berry phase, is smooth,

$$B(k) = \int_0^k dk' \frac{d}{dk'} \eta(D_{P(k')}). \quad (19)$$

The above mathematical results are consistent with the existence of \mathcal{Z}_2 obstacle found by Fu and Kane [39, 48].

B. Spectral Flow

We now study the relation between spectral flow and η -invariant. For the family of $D(k)$ with $k \in [0, \pi]$ which obeys (12), the family of eigenvalues $\lambda_P(k)$ may or may not cross the Fermi level (which is set to be zero). Define a direction of the curve $\lambda_P(k)$ which starts from $\lambda_P(0)$ and ends at $\lambda_P(\pi)$. A curve starting from $\lambda_P(0) < 0$ and ending at $\lambda_P(\pi) \geq 0$ is endowed a number $+1$ while a curve starting from $\lambda_P(0) \geq 0$ and ending at $\lambda_P(\pi) < 0$ is endowed -1 . Other curves are endowed 0. *Summation of all these number defines the spectral flow of this Dirac operator family.*

For a given $k \in [0, \pi]$, assume $\pm\epsilon \in \text{Spec } D_{P(k)}$ with $\epsilon > 0$. Then for a small interval $k \in [k_0, k_1]$, $\eta(D_{P(k)}; s)$ can be divided into two parts

$$\begin{aligned}
\eta(D_{P(k)}; s) &= \sum_{0 < |\lambda_P| < \epsilon} \text{sign}(\lambda_P) |\lambda_P|^{-s} \\
&+ \sum_{|\lambda_P| > \epsilon} \text{sign}(\lambda_P) |\lambda_P|^{-s} \\
&= \eta_{<\epsilon}(D_{P(k)}; s) + \eta_{>\epsilon}(D_{P(k)}; s),
\end{aligned} \quad (20)$$

where $\eta_{<\epsilon}(D_{P(k)}; 0)$ is a finite integer. One then has

$$\begin{aligned}
\eta_{<\epsilon}(D_{P(k_1)}; 0) - \eta_{<\epsilon}(D_{P(k_0)}; 0) &= 2\text{SF}(D_P(t))_{k \in [k_0, k_1]} \\
&+ \text{zero modes of } D_{P(k_0)} - \text{zero modes of } D_{P(k_1)}
\end{aligned} \quad (21)$$

To understand this fact, we examine the following simple example. Assuming two sets of eigenvalues

$$\begin{aligned}
&\{\lambda_1(k_0) < 0, \lambda_2(k_0) < 0, \lambda_3(k_0) = 0, \lambda_4(k_0) = 0, \lambda_5(k_0) > 0\} \\
&\{\lambda_1(k_1) < 0, \lambda_2(k_1) = 0, \lambda_3(k_1) = 0, \lambda_4(k_1) = 0, \lambda_5(k_1) > 0\},
\end{aligned}$$

the direct counting gives

$$\eta_{<\epsilon}(D_{P(k_1)}; 0) - \eta_{<\epsilon}(D_{P(k_0)}; 0) = (-1+1) - (-2+1) = 1,$$

while dimension difference of the zero modes is -1 and $2\text{SF}=2 \times 1 = 2$, which also gives 1.

Thus, we have

$$\begin{aligned}
\eta_{>\epsilon}(D_{P(k)}; s) &= \eta(D_{P(k)}; s) - \eta_{<\epsilon}(D_{P(k)}; s) \\
&= \eta(D_{P(k)}) \bmod \mathcal{Z},
\end{aligned}$$

which varies smoothly in $k \in [k_0, k_1]$. The Berry phase between $[k_0, k_1]$ is given by

$$\begin{aligned}
\int_{k_0}^{k_1} dk \frac{d}{dk} \eta(D_{P(k)}) &= \int_{k_0}^{k_1} dt \frac{d}{dt} \eta_{>\epsilon}(D_{P(k)}) \\
&= \eta_{>\epsilon}(D_{P(k_1)}) - \eta_{>\epsilon}(D_{P(k_0)}) = \eta(D_{P(k_1)}) - \eta(D_{P(k_0)}) \\
&\quad - \eta_{<\epsilon}(D_{P(k_1)}) + \eta_{<\epsilon}(D_{P(k_0)})
\end{aligned} \quad (22)$$

According to (21), one has

$$\begin{aligned}
\int_{k_0}^{k_1} dk \frac{d}{dk} \eta(D_{P(k)}) &= \eta(D_{P(k_1)}) - \eta(D_{P(k_0)}) \\
&- 2\text{SF}(D_P(t))_{k \in [k_0, k_1]} \\
&- \text{zero modes of } D_{P(k_0)} \\
&+ \text{zero modes of } D_{P(k_1)}
\end{aligned} \quad (23)$$

Dividing the interval $[0, \pi]$ into small intervals $[k_i, k_{i+1}]$ and summation over all these small intervals, we get a relation between the η -invariant and the spectral flow

$$\begin{aligned}
\tilde{\eta}(D_{P(\pi)}) - \tilde{\eta}(D_{P(0)}) &= \text{SF}(D_{P(k)})_{k \in [0, \pi]} \\
&+ \frac{1}{2} \int_0^\pi dk \frac{d}{dk} \eta(D_{P(k)}).
\end{aligned} \quad (24)$$

IV. THE SCOTT-WOJCIECHOWSKI THEOREM: AN EXPRESSION OF η -INVARIANT

If we have the whole spectrum, the η -invariant and the spectral flow can be directly read out by examining the sign of each eigenvalue as well as number of the zero modes. However, our task is to relate them with a topological invariant winding number. That is, we need to relate them to the map w given by the projection $P(k)$. The Scott-Wojciechowski theorem states a relation between ζ -function and the determinant of the map w associated with the projection P [45]. Using Eq. (16), we then set up a relation between η -invariant and the determinant of w .

A. w Map

We first rewrite the projection P . The map Q (Eq. (11)) corresponds to a projection P_Q ,

$$\begin{aligned} 0 &= P_Q \begin{bmatrix} u_{k,\alpha}^0 \\ u_{k,\alpha}^1 \\ u_{-k,\alpha}^0 \\ u_{-k,\alpha}^1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} u_{k,\alpha}^0 - Qu_{-k,\alpha}^0 \\ u_{k,\alpha}^1 - Qu_{-k,\alpha}^1 \\ u_{-k,\alpha}^0 - Qu_{k,\alpha}^0 \\ u_{-k,\alpha}^1 - Qu_{k,\alpha}^1 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 1 & 0 & -Q & 0 \\ 0 & 1 & 0 & -Q \\ -Q & 0 & 1 & 0 \\ 0 & -Q & 0 & 1 \end{bmatrix} \begin{bmatrix} u_{k,\alpha}^0 \\ u_{k,\alpha}^1 \\ u_{-k,\alpha}^0 \\ u_{-k,\alpha}^1 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} I & \Phi(P_Q) \\ \Phi(P_Q) & I \end{bmatrix} \begin{bmatrix} u_{k,\alpha} \\ u_{-k,\alpha} \end{bmatrix} \end{aligned} \quad (25)$$

and the map $P(k)$ (Eq.(12)) can be rewritten as

$$\begin{aligned} 0 &= P_\Theta \begin{bmatrix} u_{k,\alpha}^0 \\ u_{k,\alpha}^1 \\ u_{-k,\alpha}^0 \\ u_{-k,\alpha}^1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} u_{k,\alpha}^0 - e^{i\chi_{-k,\alpha}} \Theta u_{-k,\alpha}^1 \\ u_{k,\alpha}^1 + e^{i\chi_{k,\alpha}} \Theta u_{k,\alpha}^0 \\ u_{-k,\alpha}^0 - e^{i\chi_{k,\alpha}} \Theta u_{k,\alpha}^1 \\ u_{-k,\alpha}^1 + e^{i\chi_{-k,\alpha}} \Theta u_{k,\alpha}^0 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & -e^{i\chi_{-k,\alpha}} \Theta \\ 0 & 1 & e^{i\chi_{k,\alpha}} \Theta & 0 \\ 0 & -e^{i\chi_{k,\alpha}} \Theta & 1 & 0 \\ e^{i\chi_{-k,\alpha}} \Theta & 0 & 0 & 1 \end{bmatrix} \\ &\quad \times \begin{bmatrix} u_{k,\alpha}^0 \\ u_{k,\alpha}^1 \\ u_{-k,\alpha}^0 \\ u_{-k,\alpha}^1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} I & \Phi(P_\Theta, -k) \\ \Phi(P_\Theta, k) & I \end{bmatrix} \begin{bmatrix} u_{k,\alpha} \\ u_{-k,\alpha} \end{bmatrix} \end{aligned}$$

At Γ_i , note that $\Theta^\dagger = -\Theta$ and $e^{ia}\Theta = -\Theta^\dagger e^{-ia}$, $Q = 1$ and P_Θ is hermitian, i.e., $\Phi(P_\Theta, -k) = \Phi^\dagger(P_\Theta, k)$. Therefore, at Γ_i ,

$$\begin{aligned} \Phi(P_Q)\Phi^\dagger(P_\Theta) &= \begin{bmatrix} -Q & 0 \\ 0 & -Q \end{bmatrix} \begin{bmatrix} 0 & -e^{i\chi_{k,\alpha}} \Theta \\ e^{i\chi_{k,\alpha}} \Theta & 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & e^{i\chi_{k,\alpha}} \Theta \\ -e^{i\chi_{k,\alpha}} \Theta & 0 \end{bmatrix} \end{aligned}$$

On the other hand, rearranging

$$(u_{k,m}) = (u_{k,1}^0, u_{k,1}^1, \dots, u_{k,N}^0, u_{k,N}^1),$$

the map (6) reads

$$w = \begin{bmatrix} 0 & e^{i\chi_{k,1}} & 0 & \dots & 0 & 0 \\ -e^{i\chi_{-k,1}} & 0 & \dots & 0 & 0 & 0 \\ & & \dots & & & \\ 0 & 0 & 0 & \dots & 0 & e^{i\chi_{k,N}} \\ 0 & 0 & \dots & 0 & -e^{i\chi_{-k,N}} & 0 \end{bmatrix} \quad (26)$$

Thus, the map w is equivalent to the map Φ . At Γ_i , this is antisymmetric and

$$\text{Pf}[\Phi(P_Q)\Phi^\dagger(P_\Theta)(\Gamma_i)] = \text{Pf}[w(\Gamma_i)] = e^{i\sum_\alpha \chi_{k,\alpha}} \quad (27)$$

With these equations in mind, we go to the Scott-Wojciechowski theorem.

B. The Scott-Wojciechowski Theorem and Expression of η -invariant

For a smooth P , e.g., $P(k)$ we are considering, define a ζ -determinant by

$$\det_\zeta(D_P) = \begin{cases} e^{-\zeta'(D_P,0)}, & 0 \notin \text{spec } D_P \\ 0, & 0 \in \text{spec } D_P \end{cases} \quad (28)$$

where $\zeta'(D_P^2;0) = \frac{\partial}{\partial s} \zeta(D_P^2; s)|_{s \rightarrow 0}$. This is called a determinant because ζ -function is a kind of trace.

According to (16), the ζ -determinant is rewritten by

$$\det_\zeta(D_P) = e^{\frac{1}{2}(\zeta(D_P^2,0) - \eta(D_P,0)) - \frac{1}{2}\zeta'(D_P^2,0)}, \quad (29)$$

The Scott-Wojciechowski theorem [45] is stated as follows: For a smooth projection P which is of the form

$$P = \frac{1}{2} \begin{bmatrix} I & \Phi^\dagger(P) \\ \Phi(P) & I \end{bmatrix},$$

the following relation holds

$$\det_\zeta(D_P) = \det_\zeta(D_{P_C}) \det\left(\frac{I + \Phi(P_C)\Phi^\dagger(P)}{2}\right) \quad (30)$$

where the second "det" on the right hand side is the conventional determinant of an operator acting on the Hilbert space. P_C is so-called the Caldron projector which is a reference projection [44]. We do not give its definition and discuss its property because we will have a better reference projection in the present case. Also we do not explain the smooth projection. $P(k)$ we are considering are smooth.

We would like to use this theorem to express the η -invariant [44]. For the smooth projection P , $\zeta(D_P^2,0)$ is independent of the concrete form of P . Thus, in terms of (29) and assuming D_P has no zero modes [44], one has

$$\begin{aligned} e^{i\frac{\pi}{2}(\eta(D_{P_C}) - \eta(D_P))} e^{\frac{1}{2}(\zeta'(D_{P_C}^2,0) - \zeta'(D_P^2,0))} &= \frac{\det_\zeta(D_P)}{\det_\zeta(D_{P_C})} \\ &= \det\left(\frac{I + \Phi(P_C)\Phi^\dagger(P)}{2}\right). \end{aligned} \quad (31)$$

Notice that the first factor in the left hand side of the first equity is a pure phase and the second factor is real, i.e., the product of two factors can be thought as $e^{i \arg(\det)} |\det|$, i.e.,

$$\frac{\det(\frac{I+\Phi(P_C)\Phi^\dagger(P)}{2})}{|\det(\frac{I+\Phi(P_C)\Phi^\dagger(P)}{2})|} = e^{i \frac{\pi}{2}(\eta(D_{P_C})-\eta(D_P))}, \quad (32)$$

Since $\Phi(P)$ is a unitary operator, one can write $\Phi(P_C)\Phi^\dagger(P) = e^{iS}$ for $S^\dagger = S$. Then

$$\begin{aligned} \det(\frac{I+\Phi(P_C)\Phi^\dagger(P)}{2})^2 &= \det(\frac{I+e^{iS}}{2})^2 \\ &= \det(e^{iS} \cos^2 S/2) = \det(e^{iS}) \det(\cos^2 S/2) \\ &= \det(\Phi(P_C)\Phi^\dagger(P)) \det(\cos^2 S/2) \end{aligned} \quad (33)$$

For a hermitian operator S , $\det(\cos^2 S/2)$ is a positive real number. The unitary of e^{iS} means $|\det(e^{iS})| = 1$ and $\det(\Phi(P_C)\Phi^\dagger(P))$ is only a phase. Therefore,

$$\frac{\det(\frac{I+\Phi(P_C)\Phi^\dagger(P)}{2})^2}{|\det(\frac{I+\Phi(P_C)\Phi^\dagger(P)}{2})|^2} = \det(\Phi(P_C)\Phi^\dagger(P)). \quad (34)$$

Comparing (32) with (34), we have

$$e^{i\pi(\eta(D_{P_C})-\eta(D_P))} = \det(\Phi(P_C)\Phi^\dagger(P))$$

In fact, this result works for an arbitrary smooth P with η replaced by $2\tilde{\eta}$ [44]. Therefore, for a pair of smooth operators (P, Q) , one has

$$e^{2\pi i(\tilde{\eta}(D_P)-\tilde{\eta}(D_Q))} = \det(\Phi(P)\Phi^\dagger(Q)). \quad (35)$$

For P_Q and P_Θ at Γ_i , since w (or Φ) is antisymmetric,

$$e^{\pi i(\tilde{\eta}(D_{P_Q})-\tilde{\eta}(D_{P_\Theta}))} = \text{Pf}(\Phi(P_Q)\Phi^\dagger(P_\Theta)) = e^{i \sum_\alpha \chi_{k,\alpha}} \quad (36)$$

Because $Q(k=0) = Q(k=\pi) = 1$ at $t = \{0, T/2\}$, P_Q is a better reference projection than P_C . The η -invariants of P_Q vanish, i.e., $\tilde{\eta}(D_{P_Q})(0) = \tilde{\eta}(D_{P_Q})(\pi) = 0$ at $t = \{0, T/2\}$. This gives rise to, at $t = \{0, T/2\}$,

$$e^{-i\pi[\tilde{\eta}(D_{P_\Theta}(\pi))-\tilde{\eta}(D_{P_\Theta}(0))]} = e^{i \sum_\alpha (\chi_{\pi,\alpha} - \chi_{0,\alpha})} = \frac{\text{Pf}(w(\pi))}{\text{Pf}(w(0))} \quad (37)$$

Taking the logarithm both sides, one has

$$\frac{i}{\pi} \log \frac{\text{Pf}(w(\pi))}{\text{Pf}(w(0))} = (\tilde{\eta}(D_{P_\Theta}(\pi)) - \tilde{\eta}(D_{P_\Theta}(0))) \mod 2. \quad (38)$$

We will use this result later.

V. WINDING NUMBER: KANE-MELE'S INVARIANT

In Fu and Kane's work [39], Kane-Mele's invariant is defined by the change of the partial polarization, whose

topological nature is not so manifest and an additional proof was needed. In this section, we define a topological invariant winding number to identify Kane-Mele's invariant and show that this winding number is \mathbb{Z}_2 -modular to the spectral flow that we defined in Sec. III. The rigorous mathematical definition of the winding number can be found in Sec. 6 in Ref. [44].

A. Winding Number and Spectral Flow

In the previous section, we introduce a map w (or Φ) from an open path $k \in [0, \pi]$ to $U(2N)$. To define a winding number corresponding to an open path, one needs to introduce an invertible mapping f so that $f(0) = w(\pi)$ and $f(\pi) = w(0)$. For a topological insulator whose bulk states are gapped and non-degenerate, one can define an Atiyah-Patodi-Singer boundary problem so that the edge states are projection away. The solution of this boundary problem defines an invertible map f .

Now we can define a product map $w * f$ which maps $([0, \pi], [0, \pi]) \rightarrow (U(2N), U^*(2N))$ in which $U^*(2N)$ are a subset of $U(2N)$ excluding $2N \times 2N$ matrices which have eigenvalue -1 . The product map $w * f$ is a closed path and one can define a winding number in the conventional way. This winding number can be thought a winding number of an open path w and is given by [44]

$$\begin{aligned} \text{wind}(w) &= \sum_{t=0, T/2} \frac{1}{2\pi i} \left[\int_0^\pi dk \text{tr}[w^{-1}(k, t) \frac{d}{dk} w(k, t)] \right. \\ &\quad \left. - \text{tr} \log w(\pi, t) + \text{tr} \log w(0, t) \right] \\ &= \sum_{t=0, T/2} \frac{1}{2\pi i} \left[\int_0^\pi dk \text{tr}[w^{-1}(k, t) \frac{d}{dk} w(k, t)] \right. \\ &\quad \left. - 2 \log \frac{\text{Pf}(w(\pi, t))}{\text{Pf}(w(0, t))} \right] \end{aligned} \quad (39)$$

After integrating, one arrives at Eq. (8) up to a \mathbb{Z}_2 -modula.

Combining (39), (38) and (24) together, one has

$$\begin{aligned} &\left[SF(D_{P_\Theta(k)}) + \frac{1}{2} \sum_{t=0, T/2} \int_0^\pi dk \frac{d\eta(D_{P_\Theta(k)}(t))}{dk} \right] \mod 2 \\ &= \text{wind}(w) + \frac{1}{2\pi} \sum_{t=0, T/2} \int_0^\pi dk \text{tr}(w^\dagger(k, t) i \frac{d}{dk} w(k, t)). \end{aligned} \quad (40)$$

Identifying the Berry phases both sides, i.e., the integrations of continuous functions, we reach the main result

$$\text{wind}(w)_{\partial\tau_1} = \text{SF}(D_{P_\Theta}(\tau_1)) \mod 2. \quad (41)$$

The spectral flow is integer-valued. This relation shows that the winding number is indeed \mathbb{Z}_2 -valued.

B. Bulk-edge correspondence

We now explain the physical meaning of Eq. (41). The left-hand side is Kane-Mele's invariant which is a topological invariant. The right hand side says that up to an even number, Kane-Mele invariant categorizes the spectral flow of the family of Dirac operators $D_{P(k)}$.

By definition, the spectral flow counts both the discrete zero modes and the continuous gapless excitations of the system. For this spin pumping model, the edge of the system is $S^1 \times \{0\} \cup S^1 \times \{T/2\}$. In reality, we have an open boundary chain on which the ground state of this spin pumping model is not degenerate and the bulk states are fully gapped. Thus, the spectral flow counts the oriented gapless excitations, i.e., the gapless edge states in the topological insulator. The Z_2 -modula makes the direction of the edge states become not important. For the model described in Sec. II, Fu and Kane have plotted its schematic band structure in Figs. 1 and 2 of Ref. [39] in which the spectral flow of $D_{P(k)}(t)$ from $[0, \pi]$ can be read out and is indeed $+1$. By considering Kramers partner of the edge states, we explains why the parity of the number of the Kramers pairs of edge states exactly given by Kane-Mele's invariant. In this way, we understand the edge states distinguish topological insulator from conventional insulator.

VI. DISORDERS AND INTERACTIONS

As well known, weak disorder and weak interaction do not affect the topological property in quantum Hall effects. Numerical calculations [16, 17] and analytic study [18] showed that it is also the case for topological insulator. Indeed, a Kane-Mele-type Z_2 -valued topological invariant can also be defined in a disordered and interacting system [15, 39], in the spirit of the twisted boundary condition [5, 6]. In this section, we show that all results we obtained in the previous sections may also apply to the disordered and interacting systems.

Assume the wave function of the one-dimensional system with disorder obeys the twisted boundary condition,

$$\psi(x + L) = e^{i\phi} \psi(x). \quad (42)$$

This wave function is multi-valued. Making a gauge transformation

$$\chi(\phi, x) = e^{-i\phi x/L} \psi(x), \quad (43)$$

the wave function becomes a single-valued one.

The Hamiltonian with disorder then becomes $H \rightarrow H(\phi)$ as the states change. Then under the time reversal transformation,

$$\Theta H(-\phi) \Theta^{-1} = H(\phi) \quad (44)$$

Similar to the periodic case, there are four times-reversal points Γ_i . The eigen states are $|\chi(\phi, \lambda)\rangle$ with

$$H(\phi)|\chi(\phi, \lambda, \mathbf{r})\rangle = \lambda_\phi |\chi(\phi, \lambda, \mathbf{r})\rangle. \quad (45)$$

Making a substitution $(k, t) \rightarrow (\phi, t)$ and following a similar way in the previous sections, we can identify the spectral flow of the Hamiltonian family $\{H(\phi)\}$ as Kane-Mele-type invariant after modular an even integer. The correspondence between the edge states and Kane-Mele-type invariant also holds.

For an interacting system, we can use the twisted boundary condition to the many body wave function [5, 6] and the above results are still valid.

If there are the strong interaction between the edge modes, it was shown that for a topological insulator, the edge states may be gapped while the ground state may become degenerate since the time reversal symmetry is spontaneously broken [12, 13, 39]. In fact, with a generalized twisted boundary condition, a topological system has either the ground state degeneracy or gapless excitations [14].

According to the analysis given in the present work, this result is quite natural. The spectral flow of the Dirac operator family is computed by the reduced η -invariant which counts both the discrete zero modes and the gapless excitations of the system. The edge interaction, even if it is very strong, would not violate the topological nature of the system and thus the reduced η -invariant is not changed even the gapless excitations are gapped by the spontaneous or perturbative breaking of the time reversal symmetry because the zero modes, i.e., the ground state degeneracy, compensate the gapless excitations.

On the other hand, the strong bulk interaction may modify the topological classification from Z_2 invariant to a Z_8 invariant which is beyond the free fermion classifications [42]. To study these strongly interacting systems is not the goal in this work because it may require more mathematic tools such as the knowledge of the non-linear Dirac equations.

VII. COMMENTS ON HIGHER DIMENSIONAL TOPOLOGICAL INSULATORS

The concept of the spectral flow in the present work restricts to a single-parameter family of the Dirac operators. This confines the generalization of the study in this work to a higher dimensional topological insulator. For example, the correspondence $(k, t) \rightarrow (k_x, k_y)$ leads to an understanding to Kane-Mele's invariant in two spatial dimensions [39] but the spectral flow of a two-parameter Dirac operator family needs to be defined.

Mathematically, such a multi-parameter spectral flow is called *higher spectral flow* which has been introduced in Ref. [43]. Instead of the Atiyah-Patodi-Singer boundary condition problem, the problem to be solved is a (generalized) spectral section problem [49]. It has been shown that there is an index theorem in which the higher spectral flow may be expressed by the Chern character in the parameter space [43], which seems that the equivalence between two topological invariants proved in Ref. [27] is a special example of this index theorem of the Dirac op-

erator which is parameterized by the Brillouin zone. To explain these mathematical results to condensed matter physicists requires many preparations. We will present them in subsequent works.

VIII. DISCUSSIONS AND CONCLUSIONS

We studied the \mathcal{Z}_2 -modular relation between Kane-Mele's invariant in a 1+1-dimensional topological insulator and the spectral flow of a Dirac operator family of this system. This relation revealed why and in what case the edge states can categorize the topological insulators.

In fact, the index theorem associated with an Atiyah-Patodi-Singer boundary condition problem of the Dirac operator is essential to characterize the topological nature of a physical system. The topological insulators can be classified by the topological index given by the η -invariant and (higher) spectral flow. This classification is in fact closely related to other classifications of Refs. [1, 2]. The random matrix classification categorizes the topological insulators through the eigenvalues of the Hamiltonian. In the continuous limit, this yields to classify the spectrum of the Dirac operator. On the other hand, the (higher) spectral flow is in fact a repre-

sentative element of the K-group in the parameter space [43]. Therefore, our study gives an explicit representation of the classifications based on K-theory and the random matrix to the topological insulators.

Recently, there were two papers that relate the η -invariant in Atiyah-Patodi-Singer index theorems to the topological phases [50, 51]. These works are based on Dai-Freed theorem which simplifies and generalizes the gluing formula for the η -invariant [52–57]. The difficulty to calculate the integer contribution in the gluing formula in terms of this theorem was certain non-intrinsic projections are used. However, the technique used in this work is an intrinsic way to express the integer contribution by the spectral flow of a naturally defined family of self-adjoint operators [44].

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